Case Studies in Thermal Engineering 5 (2015) 114–121

Contents lists available at ScienceDirect

Case Studies in Thermal Engineering

journal homepage: www.elsevier.com/locate/csite

Molecular dynamics simulation on flow behaviors of nanofluids confined in nanochannel

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ARTICLE INFO

Article history:
Received 24 December 2014
Received in revised form
18 March 2015
Accepted 18 March 2015
Available online 20 March 2015

Keywords:
Nanofluids
Flow behaviors
Molecular dynamics simulation
Shear flow

ABSTRACT

Nanofluids are new heat transfer liquids with remarkable heat transfer capability prepared by suspending nanoparticles in traditional heat transfer liquids (water, ethylene glycol and engine oil). The key reason for the enhanced heat transfer properties of nanofluids is not only their increased thermal conductivity but also the changed rheological behavior of base fluid due to the adding of nanoparticles. However, currently the investigation into influence of shear velocity on flow behaviors of nanofluids is still inadequate. In this paper molecular dynamics simulations are used to simulate flow behaviors of nanofluids confined in nanochannel under different shear velocities. Rotation and translation of nanoparticles and nonlinear velocity profiles of nanofluids are observed. The degree of nonlinearity, as well as the rotation and translation of nanoparticles, are enhanced with the shear velocity increasing. The existence of "solid-like" absorbed layers near the plates and around the nanoparticles is also demonstrated.

1. Introduction

Nanofluids were first proposed by Choi [1] from Argonne National Laboratory in 1995. Since then, many attentions are paid to experimental and theoretical studies on heat transfer and rheological behavior of nanofluids.

Abnormal heat transfer ability of nanofluids with a very low nanoparticle concentration has been demonstrated by experimental studies. Lee et al. [2] measured thermal conductivities of oxide nanofluids by a transient hot-wire method. For the copper oxide/ethylene glycol system, thermal conductivity can be enhanced by more than 20 percent at a volume fraction of 4%. Zhang et al. [3] have observed a 27% enhancement in thermal conductivity by adding only 0.5 wt% of carbon coated Cu nanoparticles in polyethylene glycol, and 49%, 40%, and 30% enhancement in thermal conductivity for carbon coated Cu, Al, and Fe nanoparticles loading of 1.5 wt%, respectively. Xuan and Li [4] experimentally investigated convective heat transfer and flow features of Cu-water nanofluids in a tube with a constant heat flux at wall. Their results showed that the nanofluids give remarkable enhancement of heat transfer rate compared to pure water. The same conclusion has also been demonstrated by Wen et al. [5] and Heris et al. [6] with CuO-water nanofluids and Al_2O_3-water nanofluids, respectively. Rheological behavior of fluid plays a significant role in heat transfer capability. A number of researchers have studied the rheological behaviors of nanofluids experimentally. Previous studies have demonstrated that some nanofluids are

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http://dx.doi.org/10.1016/j.csite.2015.03.007
2214-157X/

Newtonian fluids in nature, and the viscosity increases with the increase of concentration of nanoparticles [7–10]. However, other nanofluids have been observed to show non-Newtonian behavior (shear-thinning behavior) [11–14]. Nusselt number and convective heat transfer coefficient of nanofluids increase with nanoparticle concentration and Reynolds number. [15–17]

Currently, there are no theoretical formulas available to predict the anomalous thermal conductivity of nanofluids satisfactorily. Researchers are attempting to find more accurate theory to predict the thermal conductivity. Yu and Choi [18,19] proposed a modified Maxwell model to include the effect of ordered nanolayer around the nanoparticles and a modified Hamilton–Crosser model for suspensions of nonspherical nanoparticles to include the effect of a solid/liquid interface. Xuan et al. [20] and Koo and Kleinstreuer [21] proposed theoretical models to predict the thermal conductivity of nanofluids including the effect of the Brownian motion of the nanoparticles. Researchers have investigated the heat transfer capability of flowing nanofluids by numerical methods such as CFD. Akbari et al. [22] compared single-phase and two-phase CFD models for the predictions of laminar mixed convection of Al_2O_3-water nanofluids. They concluded that two-phase model is more accurate for the predictions of the convective heat transfer coefficient. Namburu [23] investigated the turbulent flow and heat transfer of nanofluids and proposed that Nusselt number increases by 35% for 6% CuO nanofluids over the base fluid at a constant Reynolds number. Dawood et al. [24] reported numerical simulation for three dimensional laminar mixed convective heat transfers at different nanofluids flow in an elliptic annulus with constant heat flux. The results revealed that SiO_2-Water nanofluid has the highest Nusselt number, followed by Al_2O_3-Water, ZnO-Water, CuO-Water, and lastly pure water. The Nusselt number increased as the nanoparticle volume fraction and Reynolds number increased; however, it decreased as the nanoparticle diameter increased. Shariat et al. [25] studied laminar mixed convection Al_2O_3-water nanofluid flow in elliptic ducts with constant heat flux boundary condition employing two phase mixture model. Results showed that in a given Reynolds number (Re) and Richardson number (Ri), increasing solid nanoparticles volume fraction increases the Nusselt number (Nu) while the skin friction factor decreases. Abdolbaqi et al. [26] numerically studied heat transfer enhancement of nanofluids under turbulent flow through a straight square channel under constant heat flux conditions at the upper and lower walls. The results showed that the heat transfer rates and wall shear stress increase with an increase of the nanofluids' volume concentration. Al-Shamani et al. [27] numerical studied heat transfer due to turbulent flow of nanofluids through rib-groove channel. Their results indicated that the Trapezoidal with increasing height in the flow direction rib-trapezoidal groove has the best heat transfer rate and high Nusselt number. It is also found that the SiO_2-nanofluid has the highest value of Nusselt number in comparison with the other type of nanofluids. The Nusselt number increases as the volume fraction increases and it decreases as the nanoparticle diameter increases.

Much effort has been paid on the mechanisms of the excellent heat transfer ability by using nanofluids. Sarkar and Selvam [28] demonstrated that the thermal transport enhancement of nanofluids is mostly due to the increased movement of liquid atoms in the presence of nanoparticles and transport process for mass and heat is similar. Eapen et al. [29] showed that the thermal conductivity enhancement arises from a strong short-ranged attraction between nanoparticle and liquid. They also demonstrated that the Brownian motion of the clusters have only an insignificant role in the enhancement, which is consistent with Evans' achievement [30]. However, other researchers [31–33] reported that the Brownian motion of nanoparticles constitutes a key mechanism of the thermal conductivity enhancement. Li et al. [34] and Sachdeva and Kumar [35] showed that liquid layers around the nanoparticles lead to the more significant enhancement of the thermal conductivity of the nanofluids. But Xue et al.[36] reported that the enhancement of thermal conductivity of nanofluids cannot be explained by altered thermal transport properties of the layered simple liquid. Nie et al. [37] suggested that the thermal conductivity enhancement of nanofluids is due to the high thermal conductivity of nanoparticles themselves, but the fluid molecules make no evident contribution to the enhancement of thermal conductivity attributable to the presence of the nanoparticles at volume fractions less than 5%. Keblinski et al. [38] showed that the key factors in understanding thermal properties of nanofluids are the ballistic, rather than diffusive, nature of heat transport in the nanoparticles, combined with direct or fluid-mediated clustering effects that provide paths for rapid heat transport.

Molecular dynamics (MD) method is a computational method that solves atomic classical equations of motion with known interatomic potentials, and the physical properties can be calculated with statistical mechanics. Mohebbi conducted prediction of specific heat and thermal conductivity of nanofluids by a combined equilibrium and non-equilibrium MD simulation [39]. The results showed that the thermal conductivity increases with increasing the loadings and decreasing the temperature. They proposed that the thermal transport enhancement in nanofluid was mostly due to the increased movement of surrounding liquid phase atoms in the presence of non-metallic nanoparticle. Loulijat et al. examined the influence of solid–solid inter-atomic potential type on thermal conductivity of nanofluids by MD simulations [40]. They suggested that the thermal conductivity of (Ar–Cu) nanofluid is influenced by the type of potential used in the simulation. Sun et al. [41] focused on nanofluid's effective thermal conductivity in high-shear-rate Couette flow. It was the first attempt to calculate the thermal conductivity of shearing fluid in equilibrium molecular dynamics (EMD) method, in which transport properties are calculated by Green–Kubo formula. The nanoparticle in the nanofluid in shear field is found to rotate under the action of the velocity gradient. They have proposed that the rotation induces enhanced “microconvection” effect which is the main reason for the linear increase in the effective thermal conductivity of the shearing nanofluid with the shear rate increasing. They have also found that the increase is more sharply with lower volume fraction of nanoparticle than with higher volume fraction, because the “microconvection” effect is weakened in the nanofluid with higher volume fraction of nanoparticle resulted by the slower nanoparticle rotation speed.

The present work is designed based on the following basic understanding: the key reasons for the enhanced heat transfer

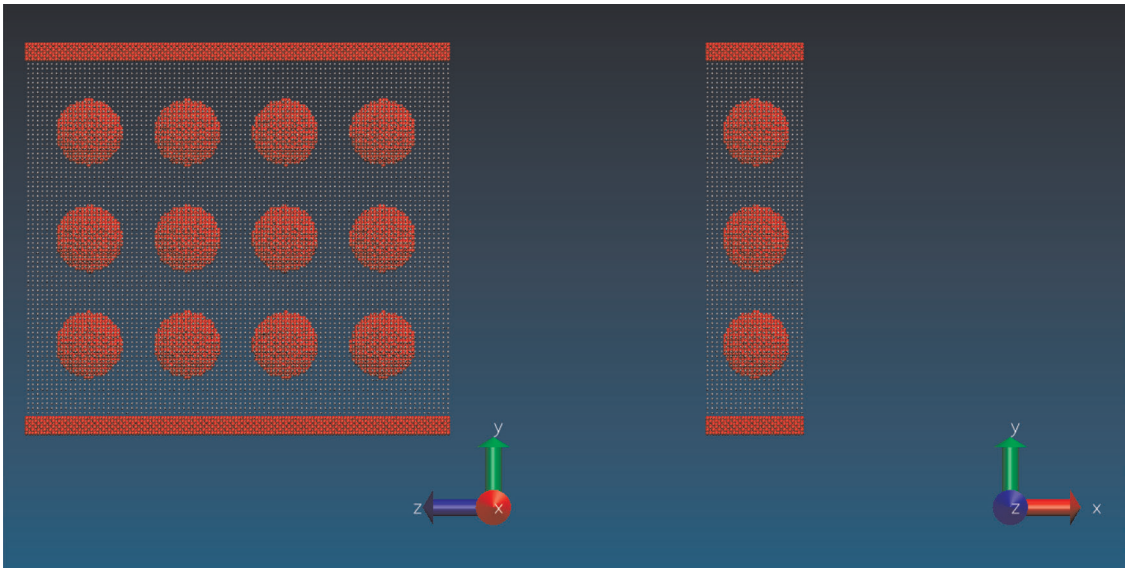

Fig. 1. Simulation model for nanofluid flow.

properties of nanofluids are not only their increased thermal conductivity but also the changed rheological behavior of base fluid due to the adding of nanoparticles. Using MD simulation, previous researchers have made achievements in studying mechanisms of conduction heat transfer in nanofluids [39–41]. However, the increased thermal conductivity of nanofluids is merely one respect of their enhanced heat transfer properties. Due to the adding of nanoparticles, rheological behavior of base fluid is also changed. The changed flow behavior with nanofluids is another important aspect for exploring the increased heat transfer properties of nanofluids.

Currently the investigation into influence of shear velocity on flow behaviors of nanofluids is still inadequate. Therefore, in this paper MD simulations are used to simulate flow behaviors of nanofluids confined in nanochannel under different shear velocities. Aiming at the flow behavior of nanofluids and motion behaviors of nanoparticles, the present MD simulation work focused on the problems that were not addressed in previous work [41], for instance, different size of the nanoparticle, different shear velocity, the influence of shear velocity on the number density, etc.

2. Simulation model

The MD simulation model is shown in Fig. 1. Between two copper plates, it is the nanofluid which is comprised of liquid argon as the base fluid with copper nanoparticles dispersed in it. There are totally 12 nanoparticles with diameter of 4 nm in the present simulation model. The simulation boxes are $5.788 \times 23.858 \times 25.846\ \mathrm{nm}^3$ in size. The thickness of each plate is $\delta = 0.904$ nm. The liquid height is $h = 22.050$ nm. Initially all the atoms of liquid argon, copper nanoparticles and plates are arranged as face-centered cubic lattice (FCC) lattices.

At this time only one vertical layer of nanoparticles is considered in the original simulation box. Periodic boundary condition (PBC) is applied in the x- and *z*-direction. By applying PBC, the original simulation box has periodic images on both sides. In the simulations, only one original simulation box needs to be concerned, and others are periodic images. During the simulation, only the properties of the original simulation box need to be recorded and propagated. The minimum-image convention is a common form of PBC particle bookkeeping in which each individual particle in the simulation interacts with the closest image of the remaining particles in the system. The use of PBC has two important reasons: (1) During the simulation, once one or more simulated particles run out of the simulation box, then there must be one or more simulated particles enter the simulation box from the adverse interface. Therefore the total simulated particle number is ensured to be a constant. (2) During the simulation, the interactions between atoms are treated by nearest image method, therefore the force on the atoms located at the boundary is comprehensive and boundary effect is eliminated. By applying PBC in the x- and *z*-direction, the simulation model in the present work is reasonable.

In our simulations, the interatomic interactions between argon atoms and those between copper and argon atoms are Lennard–Jones potential which is written as

$$U(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right], \tag{1}$$

where ε and σ are energy parameter and length scale, respectively, and r_{ij} is the intermolecular distance between atoms i

and j. For argon, $\varepsilon = 1.67 \times 10^{-21}$ J and $\sigma = 0.3405$ nm, [34] and for copper, $\varepsilon = 65.625 \times 10^{-21}$ J and $\sigma = 0.23377$ nm (Li et al. 2010). The Lorentz–Berthlot mixing rule is used to determine parameters between argon and copper atoms, [34] which are written as

$$\varepsilon_{sl} = \sqrt{\varepsilon_{ss}\,\varepsilon_{ll}}\,, \tag{2}$$

$$\sigma_{sl} = \frac{\sigma_{ss} + \sigma_{ll}}{2}, \tag{3}$$

where s and l denote solid and liquid, respectively. Therefore, it is calculated that $\varepsilon_{sl} = 10.4153 \times 10^{-21}$ J and $\sigma_{sl} = 0.2872$ nm, respectively.

Embedded atom method (EAM) potential shown in Eq. (4) is used to represent interactions between copper atoms, which is written as

$$U = \sum_i F_i\left(\sum_{j\neq i}\rho_i(\vec{r}_{ij})\right) + \frac{1}{2}\sum_{j\neq i}\phi_{ij}(\vec{r}_{ij}), \tag{4}$$

where F_i is the embedding energy which is a function of the atomic electron density ρ, ϕ is a pair potential interaction, and i and j represent atoms i and j, respectively.

The simulation time step length is 2 fs and the temperature is 86 K, at which the argon is liquid. The systems are simulated in NVT ensemble and velocity-rescale method is used to control the temperature. At first, the systems are relaxed at 86 K for 200 ps to obtain balanced states. After relaxation, only the plate temperature is controlled and the lower plate is fixed. The nanofluids model is simulated four times under different shear velocities of upper plate of 10 m/s, 30 m/s, 50 m/s and 100 m/s in z-direction, and the pure base fluid model is only simulated under the shear velocity of 50 m/s. All the simulation lengths are 10000 ps.

3. Results and discussion

Fig. 2 shows the number density profiles of fluid along y-direction under different shear velocities. In the intermediate part of the fluid regions, densities of nanofluids are larger than that of pure base fluids. This is because density of copper is larger than that of argon. When the shear velocity is 10 m/s, obvious crests and troughs of number density profiles indicate that the distribution of nanoparticles is scarcely changed by the lower shear velocity. When the shear velocity increases, the number density profiles become more uniform. This is because displacements of nanoparticles in y-direction are larger and the nanoparticle distributions are more uniform. In the vicinity of copper plates, some absorbed liquid layers are formed. The densities of layers nearest to the plates are even larger than the density of copper.

To analyze flow behaviors of nanofluids, the fluid region is divided into 125 layers along y-direction to calculate the velocity in z-direction and the fluid number density of every layer. Velocities and number densities are all averaged from 7800 ps to 9800 ps. Velocity profiles along y-direction under different shear velocities are shown in Fig. 3. It is clearly found that velocity profile of pure base fluid is linear, but velocity profiles of nanofluids are not linear. Sun et al. have reported the velocity profiles of the nanofluid with different nanoparticle volume fractions as imposed a fixed shear rate [41]. While the present work examines the velocity profiles of nanofluids with various shear velocities. And it is found that: the degree of nonlinearity increases with the increase of shear velocity. Nonlinear velocity profiles indicate that nanoparticles change the

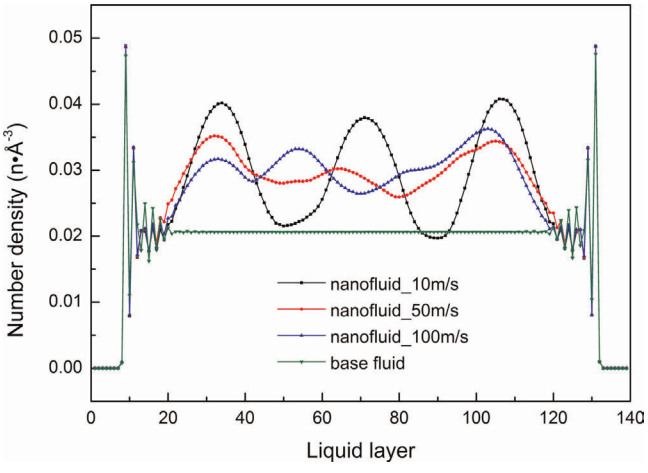

Fig. 2. Number density profiles of nanofluids and pure base fluid along y-direction.

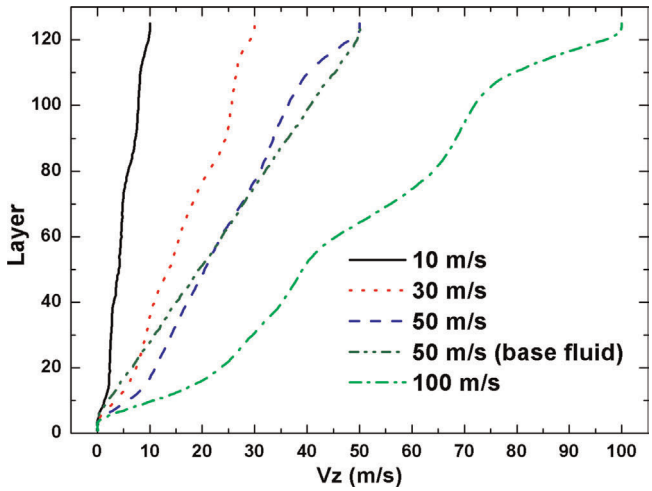

Fig. 3. Velocity profiles of nanofluids and pure base fluid along *y*-direction.

flow behaviors of fluid. From Fig. 3, it can also be observed that several layers of fluids near plates exhibit the same velocities as the plates, which indicates these layers move with the plates.

The angular velocity of nanoparticle fluctuates with simulation time as shown in Fig. 4. Angular velocity components are calculated from 200 ps to 9800 ps. The angular velocity components are averaged every 400 ps, namely, the angular velocity component quantity on 600 ps is the average from 200 ps to 600 ps, and so on. The average is over 10000 quantities which are chosen every 0.04 ps. In the figures, it is clearly found that angular velocity components around *x*-axis are obviously larger than those around *y*- and *z*-axis except for the shear velocity of 10 m/s. The nanoparticles primarily rotate around *x*-axis. Rotation around *x*-axis arises from the velocity difference between the upper and lower surface of nanoparticles, which is caused by the shear velocity. When the shear velocity is 10 m/s, angular velocities around three axes are almost the same. Rotation caused by shear velocity is unobvious. However, when the shear velocity increases, nanoparticles begin to rotate around *x*-axis obviously and fluctuations of angular velocity components around *x*-axis are intensified increasingly. Nanoparticles also rotate around *y*- and *z*-axis, and the direction of rotation changes all the time. Rotation around *y*- and *z*-axis may be caused by the complicated interaction between nanoparticles and base fluid. Rotation of nanoparticles would affect the local flow of fluid in the presence of nanoparticles and enhance local blending of nanofluids. Therefore, the velocity profiles of nanofluids are nonlinear. With the increase of shear velocity, rotation of nanoparticles become more violent, as well as the local blending effect and nonlinearity degree of velocity profile. Sun et al. has reported the average rotating speed of nanoparticle (0.553, 0.772, and 0.915 nm) [41]. In this work, larger nanoparticle (4 nm) is considered and the new outcome is: the rotating direction of nanoparticle changes all the time and the rotating speed is lower with larger nanoparticle. Furthermore, it is proposed the rotation of nanoparticles affects the local flow of fluid, further enhances local blending of nanofluids, and finally causes the nonlinearity of velocity profiles.

Nanoparticles also translate during the simulation. Fig. 5 shows the nanoparticle's translations in *x*-direction and *y*-direction, as well as the projections in x and *y*-direction, under different shear velocities. When the shear velocity is 10 m/s, translations of nanoparticles are slight, and the maximum displacement in *x*-direction is 1.809 nm and 2.400 nm in *y*-direction. However, with the increase of shear velocity, the displacements of nanoparticles become larger. When the shear velocity is 100 m/s, the maximum displacement in x- and *y*-direction is 6.487 nm and 6.064 nm, respectively. Translation of nanoparticles plays a similar role in the influence on flow behaviors as rotation. The translation also enhances the local blending effect of nanofluids. The local blending effect is intensified with the increasing shear velocity. Therefore the degree of nonlinearity of velocity profile is enhanced.

4. Conclusions

In conclusion, velocity profile of nanofluids confined in nanochannel is non-linear, and the nonlinearity of velocity profile indicates that the adding of nanoparticles changes the flow behaviors of nanofluids. Micro movements of nanoparticles (including: rotation and translation) enhance local blending of nanofluids, which cause the nonlinearity of velocity profiles. The movements of nanoparticles and nonlinearity of velocity profiles become more obvious with the increase of shear velocity. The existence of “solid-like” absorbed layers near the plates and around the nanoparticles is demonstrated. The absorbed layer exhibits higher density than the base liquid, and therefore has a higher thermal conductivity than the base liquid.

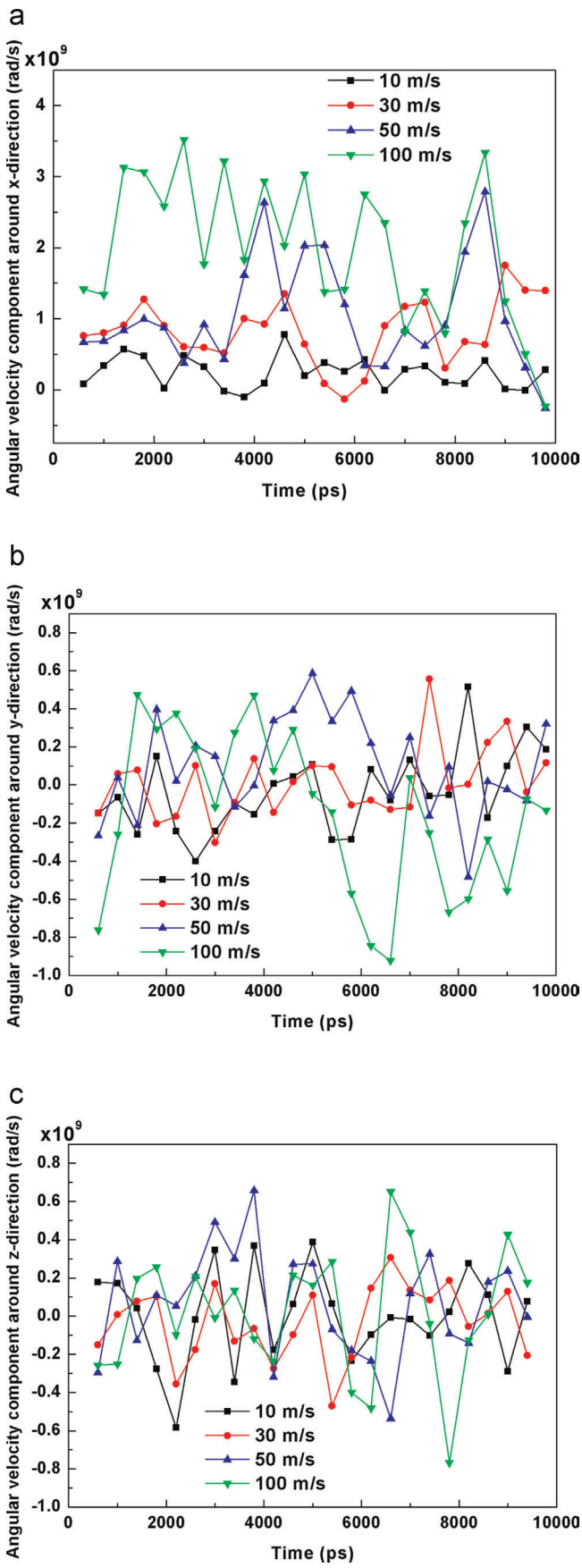

Fig. 4. Angular velocity components of nanoparticles.

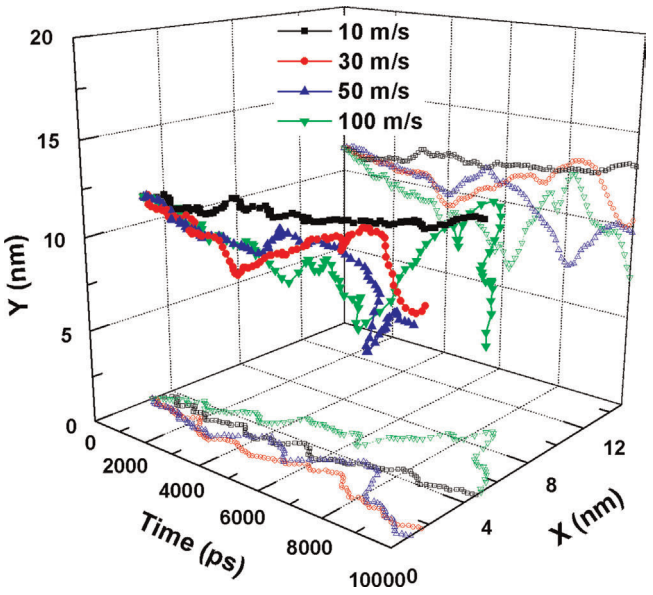

Fig. 5. Translation of nanoparticle in *x*-direction and *y*-direction.

Acknowledgments

China Postdoctoral Science Foundation funded project (Grant nos. 2014T70330 and 2013M540284). Project (HIT.NSRIF.2015116) supported by Natural Scientific Research Innovation Foundation in Harbin Institute of Technology. Project (HIT(WH)201301, HIT(WH)201406) supported by Scientific Research Foundation of Harbin Institute of Technology at Weihai.

References

[1] S.U.S. Choi, Nanofluids: from vision to reality through research, ASME J. Heat Transf., 131, , 2009, 033106.
[2] S. Lee, S.U.S. Choi, S. Li, J.A. Eastman, Measuring thermal conductivity of fluids containing oxide nanoparticles, ASME J. Heat Trans 121 (1999) 280–289.
[3] H.Y. Zhang, Q.G. Wu, J. Lin, J. Chen, Z.W. Xu, Thermal conductivity of polyethylene glycol nanofluids containing carbon coated metal nanoparticles, J. Appl. Phys. 108 (2010) 124304.
[4] Y.M. Xuan, Q. Li, Investigation on convective heat transfer and flow features of nanofluids, ASME J. Heat Trans. 125 (2003) 151–155.
[5] D. Wen, Y. Ding, Experimental investigation into convective heat transfer of nanofluids at the entrance region under laminar flow conditions, Int. J. Heat Mass Transf. 47 (2004) 5181–5188.
[6] S.Z. Heris, S.G. Etemad, A.N. Esfahany, Experimental investigation of oxide nanofluids laminar flow convective heat transfer, Int. Commun. Heat Mass 33 (2006) 529–535.
[7] R. Prasher, D. Song, J. Wang, P. Phelan, Measurements of nanofluid viscosity and its implications for thermal applications, Appl. Phys. Lett. 89 (2006) 133108.
[8] H. Chen, Y. Ding, Y. He, C. Tan, Rheological behaviour of ethylene glycol based titania nanofluids, Chem. Phys. Lett. 444 (2007) 333–337.
[9] S.K. Das, N. Putra, W. Roetzel, Pool boiling characteristics of nano-fluids, Int. J. Heat Mass Transf. 46 (2003) 851–862.
[10] N. Putra, W. Roetzel, S.K. Das, Natural convection of nano-fluids, Heat Mass Transf. 39 (2003) 775–784.
[11] P.K. Namburu, D.P. Kulkarni, D. Misra, D.K. Das, Viscosity of copper oxide nanoparticles dispersed in ethylene glycol and water mixture, Exp. Therm Fluid Sci. 32 (2007) 397–402.
[12] M. Hojjat, S.G. Etemad, R. Bagheri, J. Thibault, Turbulent forced convection heat transfer of non-Newtonian nanofluids, Exp. Therm Fluid Sci. 35 (2011) 1351–1356.
[13] M. Hojjat, S.G. Etemad, R. Bagheri, J. Thibault, Rheological characteristics of non-Newtonian nanofluids: experimental investigation, Int. Commun. Heat Mass Transf. 38 (2011) 144–148.
[14] S.Q. Zhou, R. Ni, D. Funfschilling, Effects of shear rate and temperature on viscosity of alumina polyalphaolefins nanofluids, J. Appl. Phys. 107 (2010) 054317.
[15] X.Q. Wang, A.S. Mujumdar, Heat transfer characteristics of nanofluids: a review, Int. J. Therm. Sci. 46 (2007) 1–19.
[16] L.G. Asirvatham, B. Raja, D.M. Lal, S. Wongwises, Convective heat transfer of nanofluids with correlations, Particuology 9 (2011) 626–631.
[17] S.M. Fotukian, M.N. Esfahany, Experimental study of turbulent convective heat transfer and pressure drop of dilute CuO/water nanofluid inside a circular tube, Int. Commun. Heat Mass Transf. 37 (2010) 214–219.
[18] W. Yu, S.U.S. Choi, The role of interfacial layers in the enhanced thermal conductivity of nanofluids: a renovated Maxwell model, J. Nanoparticle Res. 5 (2003) 167–171.
[19] W. Yu, S.U.S. Choi, The role of interfacial layers in the enhanced thermal conductivity of nanofluids: A renovated Hamilton-Crosser model, J. Nanoparticle Res. 6 (2004) 355–361.
[20] Y. Xuan, Q. Li, W. Hu, Aggregation structure and thermal conductivity of nanofluids, AIChE J. 49 (2003) 1038–1043.
[21] J. Koo, C. Kleinstreuer, A new thermal conductivity model for nanofluids, J. Nanoparticle Res. 6 (2004) 577–588.
[22] M. Akbari, N. Galanis, A. Behzadmehr, Comparative assessment of single and two-phase models for numerical studies of nanofluid turbulent forced convection, Int. J. Heat Fluid Flow 37 (2012) 136–146.
[23] P.K. Namburu, D.K. Das, K.M. Tanguturi, R.S. Vajjha, Numerical study of turbulent flow and heat transfer characteristics of nanofluids considering variable properties, Int. J. Thermal Sci. 48 (2009) 290–302.
[24] H.K. Dawood, H.A. Mohammed, K.M. Munisamy, Heat transfer augmentation using nanofluids in an elliptic annulus with constant heat flux boundary

condition, Case Stud. Therm Eng. 4 (2014) 32–41.
[25] M. Shariat, R.M. Moghari, A. Akbarinia, R. Rafee, S.M. Sajjadi, Impact of nanoparticle mean diameter and the buoyancy force on laminar mixed convection nanofluid flow in an elliptic duct employing two phase mixture model, Int. Commun. Heat Mass Transf. 50 (2014) 15–24.
[26] M.K. Abdolbaqi, C.S.N. Azwadi, R. Mamat, Heat transfer augmentation in the straight channel by using nanofluids, Case Stud. Therm Eng. 3 (2014) 59–67.
[27] A.N. Al-Shamani, K. Sopian, H.A. Mohammed, S. Mat, M.H. Ruslan, A.M. Abed, . Enhancement heat transfer characteristics in the channel with Trapezoidal rib–groove using nanofluids, Case Stud. Therm Eng. 5 (2015) 48–58.
[28] S. Sarkar, R.P. Selvam, Molecular dynamics simulation of effective thermal conductivity and study of enhanced thermal transport mechanism in nanofluids, J. Appl. Phys. 102 (2007) 074302.
[29] J. Eapen, J. Li, S. Yip, Mechanism of thermal transport in dilute nanocolloids, Phys. Rev. Lett. 98 (2007) 028302.
[30] W. Evans, J. Fish, P. Keblinski, Role of Brownian motion hydrodynamics on nanofluid thermal conductivity, Appl. Phys. Lett. 88 (2006) 093116.
[31] S.P. Jang, S.U.S. Choi, Role of Brownian motion in the enhanced thermal conductivity of nanofluids, Appl. Phys. Lett. 84 (2004) 4316–4318.
[32] C.H. Chon, K.D. Kihm, Empirical correlation finding the role of temperature and particle size for nanofluid (Al_2O_3) thermal conductivity enhancement, Appl. Phys. Lett. 87 (2005) 153107.
[33] P.D. Shima, J. Philip, B. Raj, Role of microconvection induced by Brownian motion of nanoparticles in the enhanced thermal conductivity of stable nanofluids, Appl. Phys. Lett. 94 (2009) 223101.
[34] L. Li, Y. Zhang, H. Ma, M. Yang, Molecular dynamics simulation of effect of liquid layering around the nanoparticle on the enhanced thermal conductivity of nanofluids, J. Nanoparticle Res. 12 (2010) 811–821.
[35] P. Sachdeva, R. Kumar, Effect of hydration layer and surface wettability in enhancing thermal conductivity of nanofluids, Appl. Phys. Lett. 95 (2009) 223105.
[36] L. Xue, P. Keblinski, S.R. Phillpot, S.U.S. Choi, J.A. Eastman, Effect of liquid layering at the liquid-solid interface on thermal transport, Int. J. Heat Mass Transf. 47 (2004) 4277–4284.
[37] C. Nie, W.H. Marlow, Y.A. Hassan, Discussion of proposed mechanisms of thermal conductivity enhancement in nanofluids, Int. J. Heat Mass Transf. 51 (2008) 1342–1348.
[38] P. Keblinski, S.R. Phillpot, S.U.S. Choi, J.A. Eastman, Mechanisms of heat flow in suspensions of nano-sized particles (nanofluids), Int. J. Heat Mass Transf. 45 (2002) 855–863.
[39] A. Mohebbi, Prediction of specific heat and thermal conductivity of nanofluids by a combined equilibrium and non-equilibrium molecular dynamics simulation, J. Mol Liq 175 (2012) 51–58.
[40] H. Loulijat, H. Zerradi, A. Dezairi, S. Ouaskit, S. Mizani, F. Rhayt, Effect of Morse potential as model of solid–solid inter-atomic interaction on the thermal conductivity of nanofluids, Adv Powder Technol ; http://dx.doi.org/10.1016/j.apt.2014.09.006. In press.
[41] C. Sun, W.Q. Lu, J. Liu, B. Bai, Molecular dynamics simulation of nanofluid's effective thermal conductivity in high-shear-rate Couette flow, Int J Heat Mass Tran 54 (2011) 2560–2567.